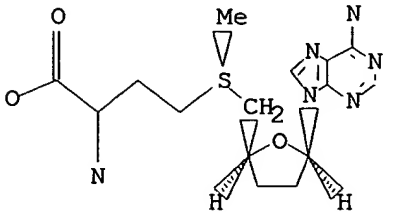
=> d his

(FILE 'HOME' ENTERED AT 15:11:23 ON 12 MAR 2003)

FILE 'REGISTRY' ENTERED AT 15:11:33 ON 12 MAR 2003
L1 STRUCTURE UPLOADED
L2 12 L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:12:17 ON 12 MAR 2003
L3 18 L2

=> d que l1
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l3 total ibib abs hitstr

L3 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:947028 CAPLUS
DOCUMENT NUMBER: 138:24947
TITLE: Chemical synthesis of S-adenosyl-L-methionine with enrichment of (S,S)-isomer
INVENTOR(S): Deshpande, Pandurang Balwant; Senthilkumar, Udayampalam Palanisamy; Padmanabhan, Ramar
PATENT ASSIGNEE(S): India
SOURCE: U.S. Pat. Appl. Publ., 10 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002188116	A1	20021212	US 2001-875044	20010607
WO 2003002588	A1	20030109	WO 2001-IN131	20010629

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

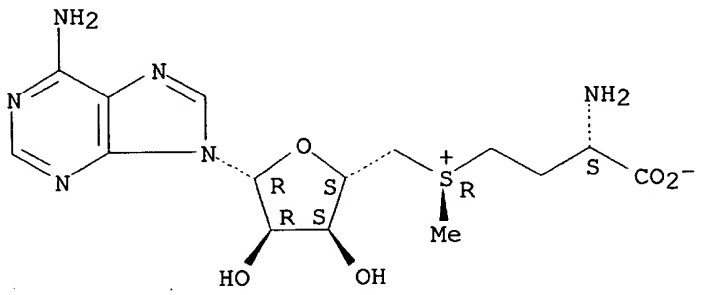
PRIORITY APPLN. INFO.: US 2001-875044 A 20010607
OTHER SOURCE(S): CASREACT 138:24947

AB The invention relates to a chem. process for the industrial manufacture of S-adenosyl-L-methionine, which consists of diastereoselective methylation of S-adenosyl-L-homocysteine with enrichment of active (S,S)-isomer. The process is simple, efficient, economical and reproducible on a large scale. Thus, trimethyloxonium tetrafluoroborate was added in lots to a solution of S-adenosyl-L-homocysteine in trifluoroacetic acid containing concentrate sulfuric acid. The mixture was maintained at -10 ± 2°C for 3.5 h to give, following workup, S-adenosyl-L-methionine (as the disulfate monotosylate salt) with 71-64% enrichment of the (S,S)-isomer.

IT **91279-78-6P 375798-66-6P**
RL: BYP (Byproduct); PREP (Preparation)
(synthesis of S-adenosyl-L-methionine by methylation of S-adenosyl-L-homocysteine)

RN 91279-78-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

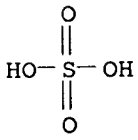
Absolute stereochemistry.



RN 375798-66-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfate (salt), 4-methylbenzenesulfonate (salt) sulfate (salt) (1:1:1:1) (9CI) (CA INDEX NAME)

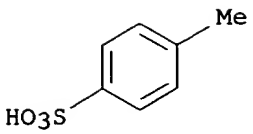
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

CRN 104-15-4
CMF C7 H8 O3 S



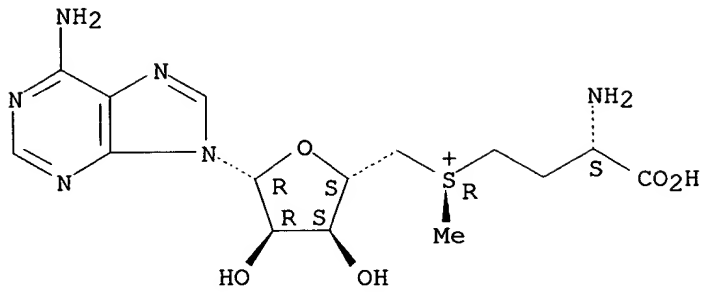
CM 3

CRN 79297-30-6
CMF C15 H23 N6 O5 S . H O4 S

CM 4

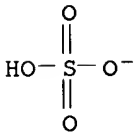
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 5

CRN 14996-02-2
CMF H O4 S



L3 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:158385 CAPLUS
DOCUMENT NUMBER: 136:205441
TITLE: Enantiomers of S-adenosyl-L-methionine
INVENTOR(S): Hebert, Rolland F.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002025926	A1	20020228	US 2001-943243	20010830

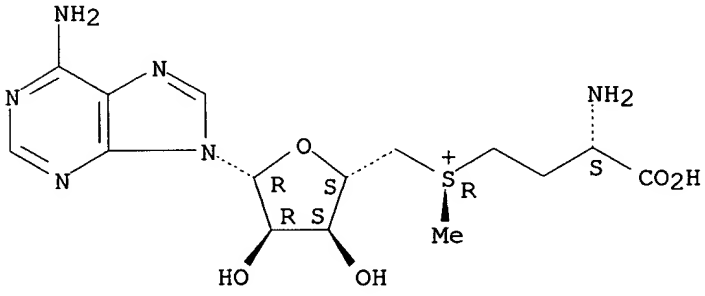
PRIORITY APPLN. INFO.: US 2000-229151P P 20000830

AB Enantiomers of S-adenosyl-l-methionine, their stable salts and their uses are described. These compns. possess potent activity in treating various conditions involving hypomethylation and transulfuration reactions and are valuable for use as active constituents in pharmaceutical compns. For example, (S,S)-S-adenosylmethionine was prepared and stabilized using p-toluene sulfonate. (S,S)-S-adenosylmethionine enteric-coated tablets (400 mg) were administered twice daily for 14 days or until remission of depression symptoms in an open, non-blind study to 10 volunteers (one patient declined to continue the study after beginning). All patients had normal results on pre-study medical examns., including laboratory examns. Eight of the nine patients who completed the trial improved over the 14 days, while one patient had no change at all. No side effects were noted or reported by any of the patients nor as measured by laboratory or phys. examination (S, S)-S-adenosylmethionine 400 mg twice daily appeared to be safe and effective in this small, non-blinded study of depression.

IT **79297-26-0 79297-28-2 79297-30-6 91279-78-6 111136-93-7 401498-62-2 401498-64-4 401498-68-8 401498-72-4 401498-79-1**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. containing enantiomers of S-adenosyl-L-methionine and their salts for therapy)

RN 79297-26-0 CAPLUS
CN Adenosine, 5'-[(3-amino-3-carboxypropyl)methylsulfonio]-5'-deoxy-, iodide, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

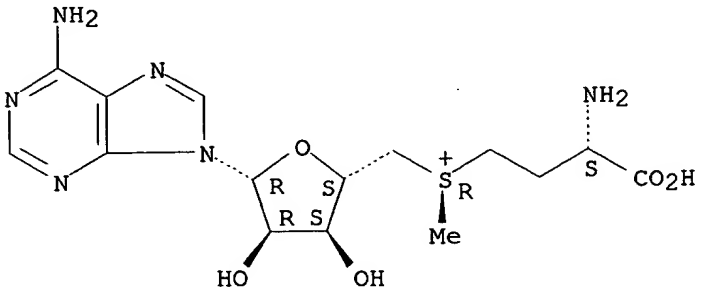
Absolute stereochemistry.



● I^-

RN 79297-28-2 CAPLUS
CN Adenosine, 5'-[(3-amino-3-carboxypropyl)methylsulfonio]-5'-deoxy-, chloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



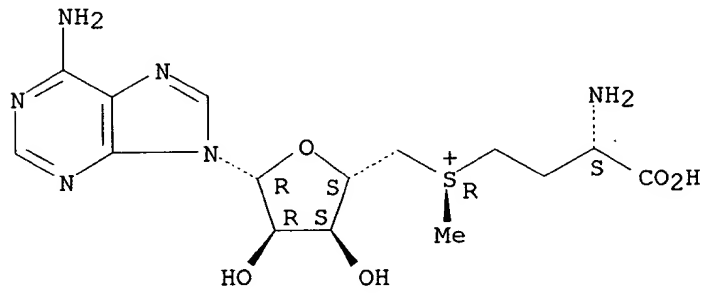
● Cl^-

RN 79297-30-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

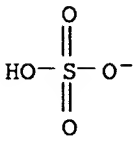
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



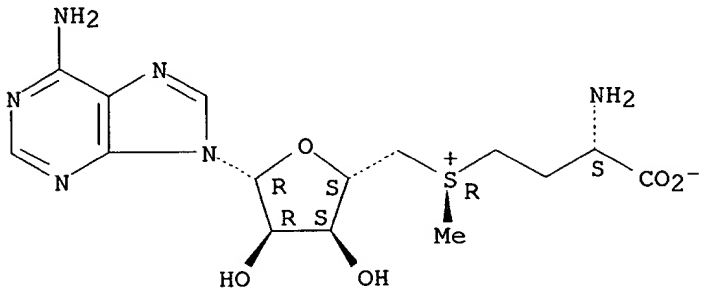
CM 2

CRN 14996-02-2
CMF H O4 S



RN 91279-78-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

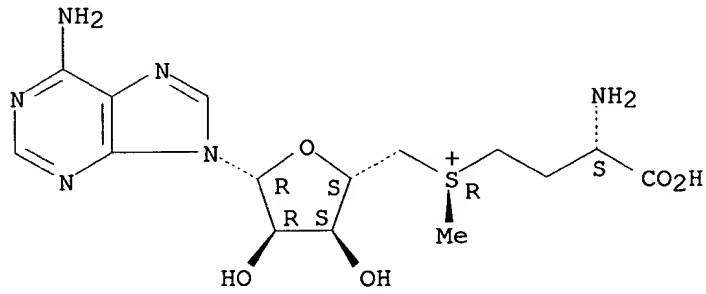


RN 111136-93-7 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

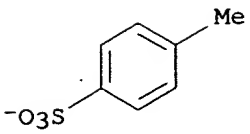
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 2

CRN 16722-51-3
CMF C7 H7 O3 S

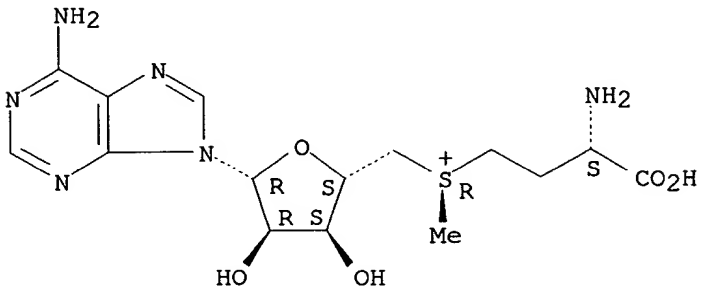


RN 401498-62-2 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfite (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

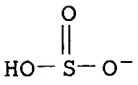
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 2

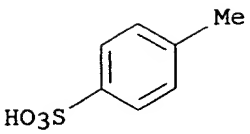
CRN 15181-46-1
CMF H O3 S



RN 401498-64-4 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, salt with 4-methylbenzenesulfonic acid (1:1), bis(4-methylbenzenesulfonate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 104-15-4
CMF C7 H8 O3 S



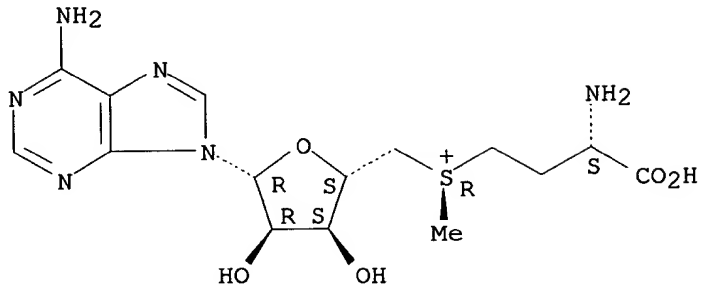
CM 2

CRN 111136-93-7
CMF C15 H23 N6 O5 S . C7 H7 O3 S

CM 3

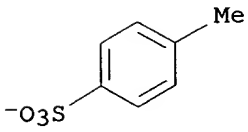
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 4

CRN 16722-51-3
CMF C7 H7 O3 S

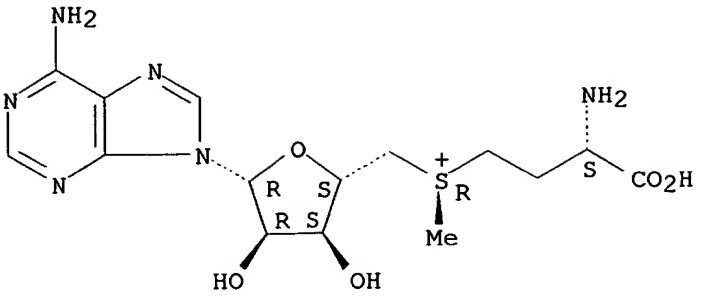


RN 401498-68-8 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, carbonate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

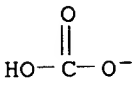
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



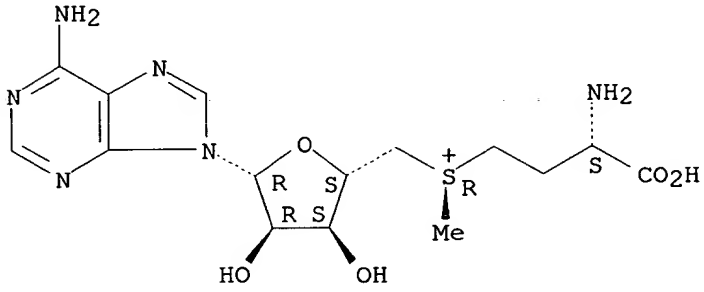
CM 2

CRN 71-52-3
CMF C H O3



RN 401498-72-4 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

RN 401498-79-1 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, 1,2-ethanedisulfonate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

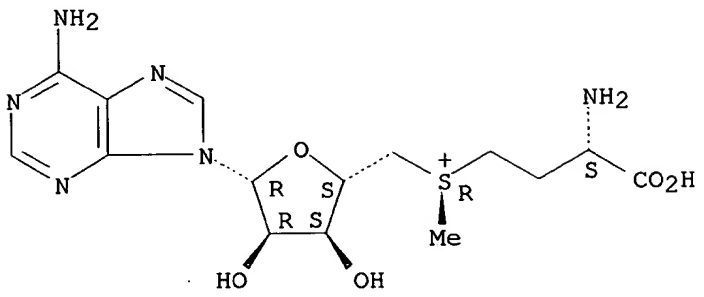
CRN 147679-24-1
CMF C2 H5 O6 S2

$HO_3S-CH_2-CH_2-SO_3^-$

CM 2

CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



L3 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:868476 CAPLUS
DOCUMENT NUMBER: 136:5067
TITLE: Process for the preparation of pharmaceutically acceptable salts of (SS-RS)-S-adenosyl-L-methionine
INVENTOR(S): Berna, Marco; Sivieri, Lino; Santambrogio, Gianni; Valoti, Ermanno
PATENT ASSIGNEE(S): Chementecno S.r.l., Italy
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090130	A1	20011129	WO 2001-EP3633	20010330
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1283845	A1	20030219	EP 2001-943206	20010330
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002010147	A1	20020124	US 2001-829906	20010411
US 2002173012	A1	20021121	US 2002-142876	20020513

PRIORITY APPLN. INFO.: IT 2000-MI1158 A 20000525

WO 2001-EP3633 W 20010330
US 2001-829906 A3 20010411

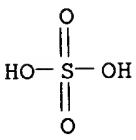
AB The present invention relates to a process for the preparation of pharmaceutically acceptable salts of (SS,RS)-S-adenosyl-L-methionine and allows one to obtain the salified (RS)-(+)-S-adenosyl-L-methionine diastereoisomer in amts. ≤3% with respect to the salified (SS)-(+)-S-adenosyl-L-methionine diastereoisomer; the salts that can be obtained by the process of the invention keep their configuration stable in time.

IT **375798-66-6P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(process for the preparation of pharmaceutically acceptable salts of (SS-RS)-S-adenosyl-L-methionine)

RN 375798-66-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfate (salt), 4-methylbenzenesulfonate (salt) sulfate (salt) (1:1:1:1) (9CI) (CA INDEX NAME)

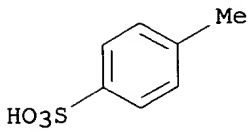
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

CRN 104-15-4
CMF C7 H8 O3 S



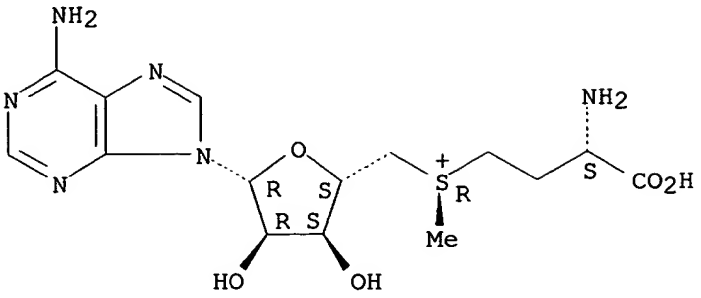
CM 3

CRN 79297-30-6
CMF C15 H23 N6 O5 S . H O4 S

CM 4

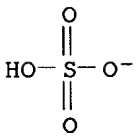
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



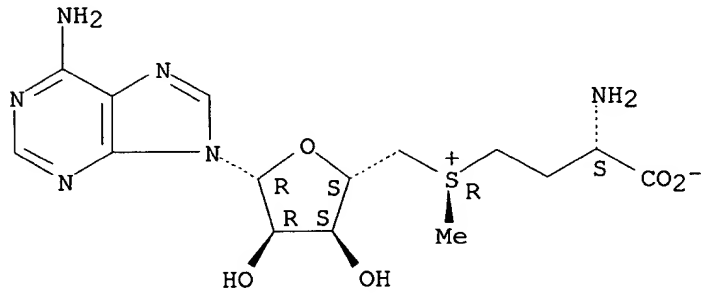
CM 5

CRN 14996-02-2
CMF H O4 S



IT **91279-78-6**
RL: REM (Removal or disposal); PROC (Process)
(process for the preparation of pharmaceutically acceptable salts of (SS-RS)-S-adenosyl-L-methionine)
RN 91279-78-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:680323 CAPLUS
DOCUMENT NUMBER: 135:368482
TITLE: Glutamate 47 in 1-Aminocyclopropane-1-carboxylate

Synthase Is a Major Specificity Determinant

AUTHOR(S): McCarthy, Darla L.; Capitani, Guido; Feng, Liang; Gruetter, Markus G.; Kirsch, Jack F.

CORPORATE SOURCE: Department of Molecular and Cell Biology Division of Biochemistry and Molecular Biology, University of California, Berkeley, CA, 94720-3206, USA

SOURCE: Biochemistry (2001), 40(41), 12276-12284.
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

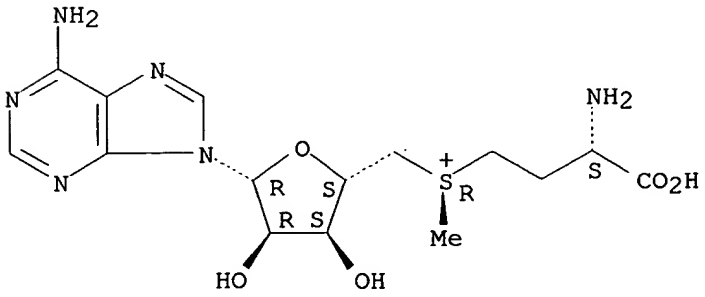
AB Glutamate 47 is conserved in 1-aminocyclopropane-1-carboxylate (ACC) synthases and is positioned near the sulfonium pole of (S,S)-S-adenosyl-L-methionine (SAM) in the modeled pyridoxal phosphate quinonoid complex with SAM. E47Q and E47D constructs of ACC synthase were made to investigate a putative ionic interaction between Glu47 and SAM. The kcat/Km values for the conversion of (S,S)-SAM to ACC and methylthioadenosine (MTA) are depressed 630- and 25-fold for the E47Q and E47D enzymes, resp. The decreases in the specificity consts. are due to redns. in kcat for both mutant enzymes, and a 5-fold increase in Km for the E47Q enzyme. Importantly, much smaller effects were observed for the kinetic parameters of reactions with the alternate substrates L-vinylglycine (L-VG) (deamination to form α-ketobutyrate and ammonia) and L-alanine (transamination to form pyruvate), which have uncharged side chains. L-VG is both a substrate and a mechanism-based inactivator of the enzyme, but the partition ratio, kcat/kinact, is unaffected by the Glu47 mutations. ACC synthase primarily catalyzes the β,γ-elimination of MTA from the (R,S) diastereomer of SAM to produce L-VG, but catalyzes the formation of ACC to a lesser extent via α,γ-elimination of MTA. The partition ratios for (α,γ/β,γ)-elimination on (R,S)-SAM are 0.4, ≤0.014, and ≤0.08 for the wild-type, E47Q, and E47D enzymes, resp. The results of these expts. strongly support a role for Glu47 as an anchor for the sulfonium pole of (S,S)-SAM, and consequently a role as an active site determinant of reaction specificity.

IT **60018-86-2**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Glu47 in 1-aminocyclopropane-1-carboxylate synthase is a major specificity determinant)

RN 60018-86-2 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:283779 CAPLUS
DOCUMENT NUMBER: 134:300801
TITLE: Nutraceutical products containing S-adenosyl-L-methionine and dietary supplements
INVENTOR(S): Howard, Larry
PATENT ASSIGNEE(S): Pharmnseas, Inc., USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001026646	A1	20010419	WO 2000-US27559	20001006

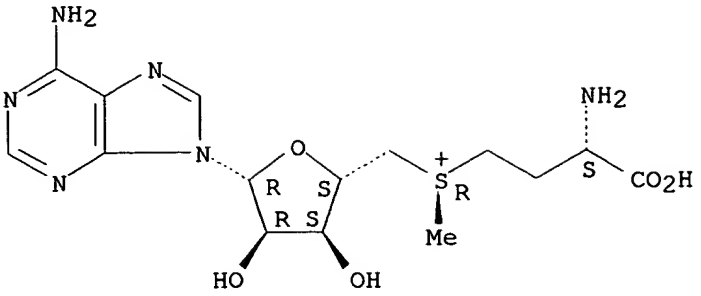
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 1999-158298P P 19991008
US 1999-158328P P 19991008
US 1999-158329P P 19991008
US 1999-158480P P 19991008
US 1999-158482P P 19991008

AB A nutraceutical product comprises a mixture S-adenosyl-L-methionine (SAMe) and a dietary supplement, where the moisture content of the product is <5% by weight A nutraceuticallly preferred product includes a mixture of (RS)-(+)-SAMe and (SS)-(+)-SAMe diastereoisomers, with the (SS)-(+)-SAMe diastereoisomer being at a concentration of at least 95% of the mixture Thus, a composition contained Kava Kava containing 30% kavalactones 35.3, SAMe tosylate salt 47.1, Valerian 5.9, excipients and fillers 200 kg and was filled into capsules.

IT **60018-86-2**
RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nutraceutical products containing adenosylmethionine and dietary supplements)
RN 60018-86-2 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:634592 CAPLUS
DOCUMENT NUMBER: 129:339812
TITLE: Evidence that S-adenosyl-L-methionine diastereoisomers may reduce ischemia-reperfusion injury by interacting with purinoceptors in isolated rat liver
AUTHOR(S): Dunne, J. Bruce; Alexander, Barry; Williams, Roger; Tredger, J. Michael
CORPORATE SOURCE: Institute of Liver Studies, Academic Department of Surgery, King's College Hospital and School of Medicine and Dentistry, London, SE5 9PJ, UK
SOURCE: British Journal of Pharmacology (1998), 125(1), 225-233
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mechanisms underlying the hemodynamic activity of diastereoisomers of S-adenosyl-L-methionine (SAM) were investigated using inhibitors of purinoceptors and nitric oxide (NO) synthase in perfused rat livers damaged by sequential 24 h cold and 20 min rewarming ischemia + reperfusion. Stored livers were flushed with 10 mL saline alone (control) or with added (R,S) or (S,S) SAM (100 μM) and reperfused in the absence (control) or presence of 10 μM 8-phenyltheophylline (8-PT) or 100 μM L-N-monomethylarginine (L-NMMA). Both SAM diastereoisomers rapidly increased blood flow and bile production vs. controls ($P<0.001$) but the (R,S) isomer induced greater increases in blood flow and the (S,S) isomer greater increases in bile production: 625 vs. 596 vs. 518 mL blood flow and 100 vs. 119 vs. 56 mg bile production per g liver over 3 h in (R,S), (S,S) and control, resp. 8-PT prevented the enhancement of blood flow by (S,S) SAM (529 vs. 596 mL g-1 liver over 3 h for (S,S) SAM alone, $P<0.001$), but was without effect in control livers. 8-PT also reduced SAM-enhanced bile production: 51 vs. 119 mg g-1 liver over 3 h, $P<0.001$. L-NMMA reduced blood flow and bile production similarly in the absence or presence of (S,S) SAM. Thus, SAM may improve liver perfusion after ischemia-reperfusion injury via stimulation of P1 (A2) purinoceptors at which SAM shows activity. The choleretic activity of (S,S) SAM is disproportionately greater than enhanced blood flow and may occur independently of a NO-dependent component of bile production

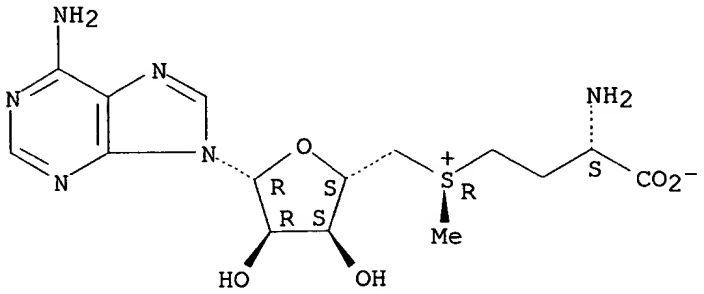
IT **91279-78-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)
(evidence that S-adenosyl-L-methionine diastereoisomers may reduce ischemia-reperfusion injury by interacting with purinoceptors in isolated rat liver)

RN 91279-78-6 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:967494 CAPLUS

DOCUMENT NUMBER: 124:45748

TITLE: Preparation of 5-deoxy-5-alkylthio-D-riboses and active oxygen eliminating agents containing them

INVENTOR(S): Kiuchi, Koji; Kumai, Juji; Morishige, Nada; Shiozaki, Shozo; Ando, Koichi

PATENT ASSIGNEE(S): Nippon Zeon Co, Japan; Kagaku Gijutsucho Hoshasen Iga

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

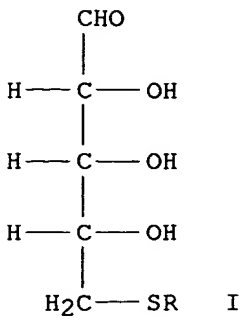
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07238023	A2	19950912	JP 1994-52763	19940225

PRIORITY APPLN. INFO.: JP 1994-52763 19940225

OTHER SOURCE(S): MARPAT 124:45748

GI



I

AB Active O eliminating agents containing the title compds. I (R = C1-6 linear or branched alkyl) or their pharmacol. acceptable salts are claimed. The agents show cytoprotective action against radiation and are useful for prevention of peroxidn. of membrane lipids, inflammation, aging, ischemic diseases, carcinogenesis, diabetes mellitus, cataract, emphysema, parkinsonism, radiation disorders caused from active O species. I.p. administration of I (R = Me) (II) (preparation given) to mice before irradiation with γ-ray significantly expanded survival rate. II showed high scavenging effect to OH radical in vitro.

IT **111136-93-7P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(deoxy(methylthio)adenosine from; active O eliminating agents containing deoxy(alkylthio)riboses for prevention of radiation disorders and other diseases)

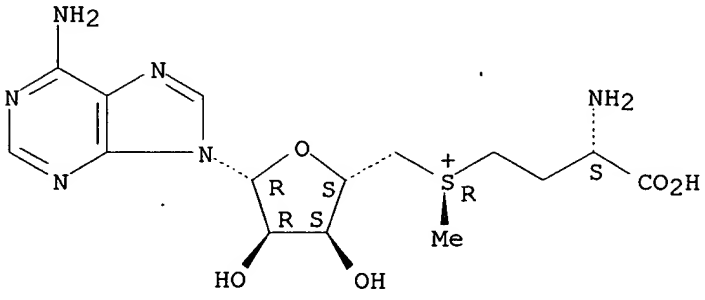
RN 111136-93-7 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60018-86-2
CMF C15 H23 N6 O5 S

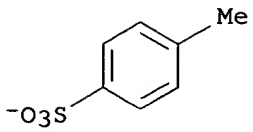
Absolute stereochemistry.



CM 2

CRN 16722-51-3

CMF C7 H7 O3 S

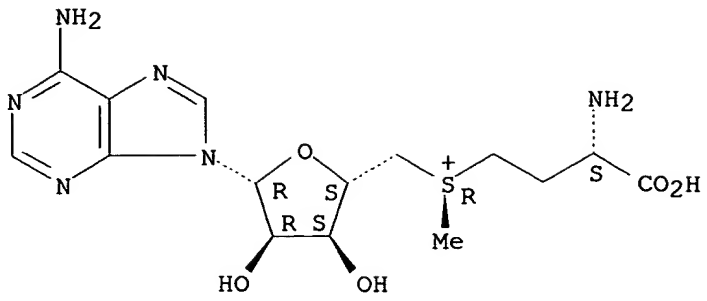


L3 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:449524 CAPLUS
DOCUMENT NUMBER: 122:248491
TITLE: Stability-indicating proton nuclear magnetic resonance spectroscopic method for determination of S-adenosyl-L-methionine in tablets
AUTHOR(S): Revelle, Larry K.; d'Avignon, D. Andre; Reepmeyer, John C.; Zerfing, Richard C.
CORPORATE SOURCE: Div. Drug Anal., U.S. Food Drug Administration, St. Louis, MO, 63101, USA
SOURCE: Journal of AOAC International (1995), 78(2), 353-8
CODEN: JAINEE; ISSN: 1060-3271
PUBLISHER: AOAC International
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We present a simple, accurate, stability-indicating NMR (NMR) method for determining active (S,S) and inactive (R,S) epimers of S-adenosyl-L-methionine (SAM) in tablets. The SCH3 resonances of SAM epimers were well resolved at 300 MHz. Individual essays of 5 SAM tablets gave SAM values of 101.3±1.7% of declared amts. Tablet solns. were assayed at a level of 8.0 mg/mL, but the method was linear for SAM concns. ranging from 64 to 1 mg/mL (correlation coefficient, 0.9996). Reproducibility was indicated by a relative standard deviation of 0.33% for 6 replicate essays for total SAM at a concentration of 8 mg/mL. In contrast to the proprietary liquid chromatog. (LC) method, which requires SAM as an external standard, the NMR method uses sodium trimethylsilylpropionate-d4 (TSP) both as an internal standard and as a chem. shift reference The method was used to test the stability of SAM analytes under various pH levels and temps. We found 8% inactivation of SAM due to epimerization over a 24 h period at room temperature and pH 5. SAM solns. showed no detectable inactivation after 14 days when stored below 0°C.

IT **60018-86-2**
RL: ANT (Analyte); ANST (Analytical study)
(determination of S-adenosyl-L-methionine in tablets by NMR)
RN 60018-86-2 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



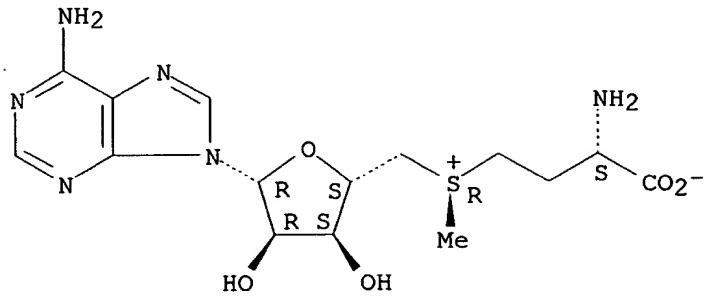
L3 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:135028 CAPLUS
DOCUMENT NUMBER: 112:135028
TITLE: The specificity of interaction between S-adenosyl-L-methionine and a nucleolar 2'-O-methyltransferase
AUTHOR(S): Segal, David M.; Eichler, Duane C.
CORPORATE SOURCE: Coll. Med., Univ. South Florida, Tampa, FL, 33612, USA
SOURCE: Archives of Biochemistry and Biophysics (1989), 275(2), 334-63
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structural features of S-adenosyl-L-methionine (SAM) required for optimal binding to a nucleolar RNA 2'-O-methyltransferase were elucidated using various analogs of SAM with modifications of the amino acid, sugar, sulfonium center, and base portions of the mol. Equilibrium binding consts. for SAM and each analog were determined by a nitrocellulose filter binding assay. To ensure the chiral and chem. purity of the 3H-labeled SAM used in the binding expts., a cation-exchange HPLC procedure was developed to sep. degradation products of SAM such as adenine and 5'-deoxy-5'-methylthioadenosine, as well as to sep. the (S,S)-SAM from the biol. inactive (R,S)-SAM stereoisomer. S-Adenosyl-L-homocysteine, a product of the methyltransferase reaction, bound equally as well as (S,S)-SAM, indicating that neither the charge nor the Me group at the sulfonium center of (S,S)-SAM is essential for maximal binding. Other modifications of the sulfonium center demonstrated that an S to C atom replacement had little effect on binding affinity, whereas substituting an Et group for the Me group greatly reduced the binding affinity. In addition, the chirality at the sulfonium center was important. The naturally occurring S-chiral form had a 10-fold higher binding affinity than the R-chiral form. No significant stereospecificity was observed relative to the chiral α-C of the methionine moiety in SAM. The α-amino group of methionine and the 6-amino group of adenine were both required for maximal binding, whereas the loss of the 2'-hydroxyl group on the ribose moiety was not. Taken together, these results defined some of the specific geometric and functional group requirements which affect the specificity of interaction between S-adenosyl-L-methionine and the nucleolar 2'-O-methyltransferase.

IT **91279-78-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction stereospecificity with RNA methyltransferase of nucleolus)
RN 91279-78-6 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

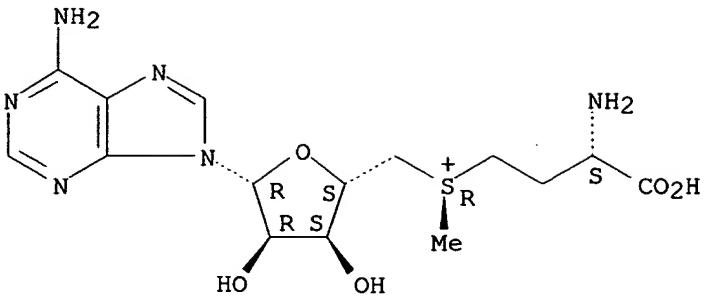


L3 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:435586 CAPLUS
DOCUMENT NUMBER: 111:35586
TITLE: Specificity of S-adenosyl-L-methionine in the inactivation and the labeling of 1-aminocyclopropane-1-carboxylate synthase isolated from tomato fruits
AUTHOR(S): Satoh, Shigeru; Yang, Shang Fa
CORPORATE SOURCE: Dep. Biol. Sci., Tohoku Univ., Sendai, 980, Japan
SOURCE: Archives of Biochemistry and Biophysics (1989), 271(1), 107-12
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1-Aminocyclopropane-1-carboxylase (ACC) synthase (I), which catalyzes the conversion of S-adenosyl-L-methionine (AdoMet) to ACC, is irreversibly inactivated by its substrate, AdoMet. AdoMet has 2 diastereomers with respect to its sulfonium center, (-)-Ado-Met and (+)-AdoMet. The (+)- and (-)-AdoMet isomers were prepared from a com. source, and their activities as a substrate and as an inactivator of ACC synthase isolated from tomato fruits were compared. Only (-)-AdoMet produced ACC, whereas both (-)- and (+)-AdoMet inactivated I; (+)-AdoMet inactivated I 3-fold faster than (-)-AdoMet. Previously, it was shown that I was specifically radiolabeled when the enzyme was incubated with S-adenosyl-L-[3,4-14C]methionine. The present results further indicated that S-adenosyl-L-[carboxyl-13C]methionine, but not S-adenosyl-L-[methyl-14C]methionine, radiolabeled I. The data suggested that the 2-aminobutyric acid portion of AdoMet is linked to I during the autoinactivation process. A possible mechanism for I inactivation by AdoMet was discussed.

IT **79297-28-2**
RL: BIOL (Biological study)
(aminocyclopropanecarboxylate synthase inhibition by)
RN 79297-28-2 CAPLUS
CN Adenosine, 5'-[(3-amino-3-carboxypropyl)methylsulfonio]-5'-deoxy-, chloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



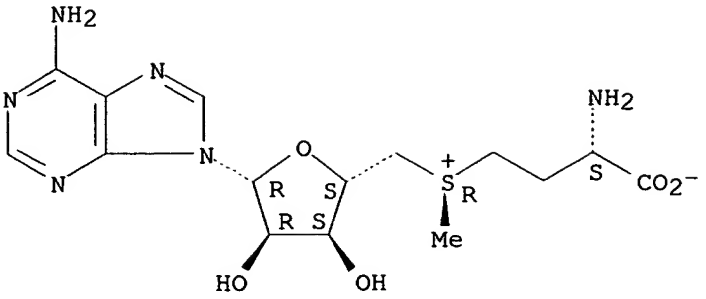
● Cl^-

L3 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:3615 CAPLUS
DOCUMENT NUMBER: 110:3615
TITLE: Stereochemistry of enzymic formation of the berberine bridge in protoberberine alkaloids
AUTHOR(S): Frenzel, Thomas; Beale, John M.; Kobayashi, Motomasa; Zenk, Meinhart H.; Floss, Heinz G.
CORPORATE SOURCE: Inst. Pharm. Biol., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1988), 110(23), 7878-80
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:3615

AB Using the individual purified enzymes, the stereochem. fate of a chiral Me group from S-adenosyl-L-methionine (AdoMet) was traced through the reaction sequence leading to the formation and subsequent dehydrogenation of the berberine bridge in the biosynthesis of protoberberine alkaloids. The steric course of the individual steps was ascertained by chem. degradation and chirality anal. of the recovered Me groups, by 3H NMR spectroscopy, and by following 3H release into solvent. The results showed that (1) the Me group of AdoMet was transferred to the N atom of norreticuline with inversion of configuration, (2) berberine bridge enzyme cyclized reticuline by abstracting an N-Me H atom with kH/kD .apprx. 4 and replacing it with the Ph group in an inversion mode, and (3) S-tetrahydroprotoberberine oxidase dehydrogenated scoulerine with nonstereospecific H atom removal from C-8, suggesting that only the 1st half-reaction of this conversion is enzyme-mediated.

IT **91279-78-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with norreticuline Me transferase)
RN 91279-78-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

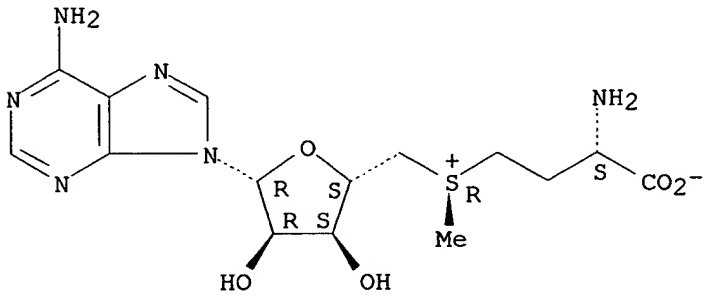


L3 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:613991 CAPLUS
DOCUMENT NUMBER: 107:213991
TITLE: Alternate substrates and inhibitors of 1-aminocyclopropane-1-carboxylic acid synthase
AUTHOR(S): Khani-Oskouee, Shahrokh; Ramalingam, Kondareddiar; Kalvin, Douglas; Woodard, Ronald W.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA
SOURCE: Bioorganic Chemistry (1987), 15(2), 92-9
CODEN: BOCMBM; ISSN: 0045-2068
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Structural analogs of (-)-S-adenosyl-L-methionine (SAM), in which the heterocyclic base was modified, were used to elucidate the active site conformation of the enzyme 1-aminocyclopropane-1-carboxylic acid (ACC) synthase, which was partially purified from Lycopersicon esculentum (tomato). These potential substrate analogs were screened for activity both as substrates and(or) as inhibitors of ACC synthase. In general, ACC synthase had a rather rigid specificity for the structural features of the natural substrate (SAM), in that only the purine base adenosine and adenosine analogs in which the N6 atom was modified were substrates.

IT **91279-78-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction kinetics with aminocyclopropane carboxylate synthase of tomato)
RN 91279-78-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:598873 CAPLUS
DOCUMENT NUMBER: 107:198873
TITLE: S-Adenosylmethionine: stability and stabilization
AUTHOR(S): Matos, Jose R.; Wong, Chi Huey
CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SOURCE: Bioorganic Chemistry (1987), 15(1), 71-80
CODEN: BOCMBM; ISSN: 0045-2068
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A kinetic study was carried out on the stability of (-)-S-adenosylmethionine [(-)-I] in solution to decomposition and epimerization, using a HPLC technique for the separation of both (+)- and (-)-I and 1H NMR anal. of the epimeric S-CH3 chem. shifts. The results obtained from the effects of pH, temperature, and sulfonium counterions on the stability of I indicate that the epimerization proceeds through pyramidal inversion of the sulfonium pole. The optimal conditions for I be stable in solution to decomposition and epimerization is to keep the compound at pH 3-5, containing an excess of large-size, nonnucleophilic counterions such as tosylate or sulfate.

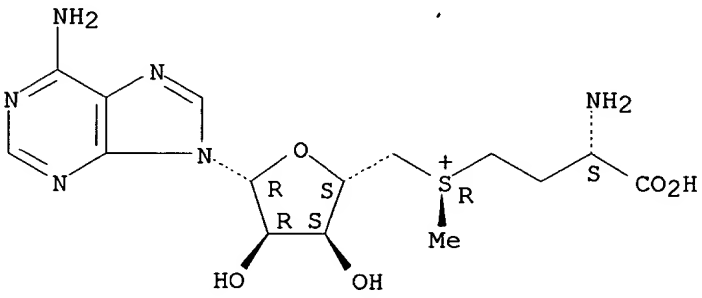
IT **79297-30-6 111136-93-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(decomposition or epimerization of, kinetics of)

RN 79297-30-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

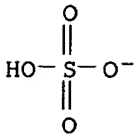
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 2

CRN 14996-02-2
CMF H O4 S

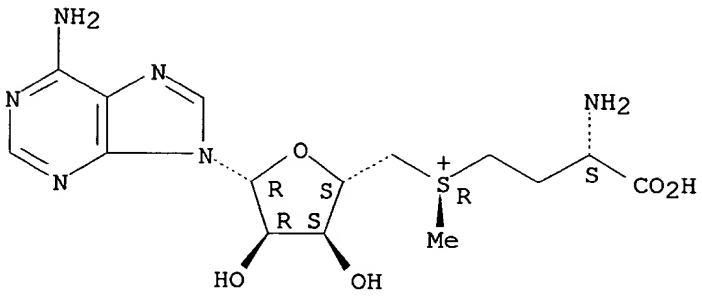


RN 111136-93-7 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

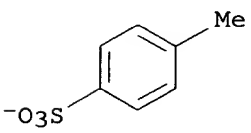
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.



CM 2

CRN 16722-51-3
CMF C7 H7 O3 S



L3 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:456829 CAPLUS
DOCUMENT NUMBER: 105:56829
TITLE: Chromatographic analysis of the chiral and covalent instability of S-adenosyl-L-methionine
AUTHOR(S): Hoffman, Jerald L.
CORPORATE SOURCE: Health Sci. Cent., Univ. Louisville, Louisville, KY, 40292, USA
SOURCE: Biochemistry (1986), 25(15), 4444-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

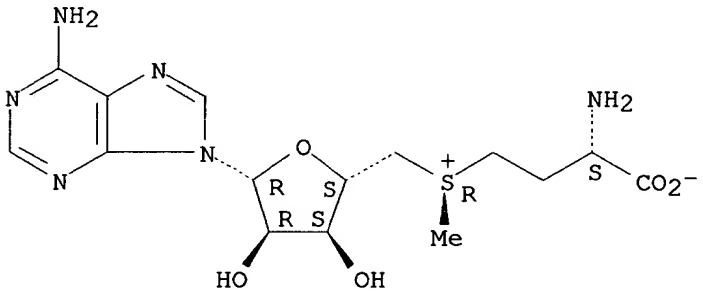
AB A cation-exchange HPLC method is described for separating (S,S)-AdoMet (where the designations refer to the S and the α-C atoms, resp.) from the biol. inactive (R,S)-AdoMet that results from racemization at the S atom. This method was used to measure the rates of the degradation reactions of (S,S)-AdoMet as a function of pH. These reactions and the 1st-order rate consts., which were found at 37° and pH 7.5, were: racemization, 1.8 + 10-6 s-1; cleavage to homoserine lactone and 5'-(methylthio)adenosine, 4.6 + 10-6 s-1; and hydrolysis to adenine and S-pentosylmethionine, 3 + 10-6 s-1. Racemization showed no change in rate over the pH range 7.5-1.5. The cleavage reaction persisted until the pH was lowered to 1.5, but hydrolysis ceased at pH 6. Com. samples of nonradioactive AdoMet contained 20-30% (R,S)-AdoMet, whereas a sample of [methyl-3H]AdoMet had <1% (R,S)-AdoMet. Preparing enzyme substrates by mixing such samples will cause an underestimate of specific activity and an overestimate of the amount of product. The (R,S)-AdoMet/(S,S)-AdoMet ratio in mouse liver was 0.03, much less than the value of 0.19 calculated from the above rate consts. An enzyme extract from mouse liver did not degrade (R,S)-AdoMet, but a more thorough search may find such an activity. In any event, the cleavage and hydrolysis reactions partially balance the racemization of (S,S)-AdoMet in vivo and prevent excessive accumulation of (R,S)-AdoMet.

IT **91279-78-6**
RL: PROC (Process)
(resolution of, by HPLC)

RN 91279-78-6 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1984:468349 CAPLUS

DOCUMENT NUMBER: 101:68349

TITLE: Stereochemical course of the biosynthesis of 1-aminocyclopropane-1-carboxylic acid. I. Role of the asymmetric sulfonium pole and the α-amino acid center

AUTHOR(S): Khani-Oskouee, Shahrokh; Jones, Jeffrey P.; Woodard, Ronald W.

CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109, USA

SOURCE: Biochemical and Biophysical Research Communications (1984), 121(1), 181-7

CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

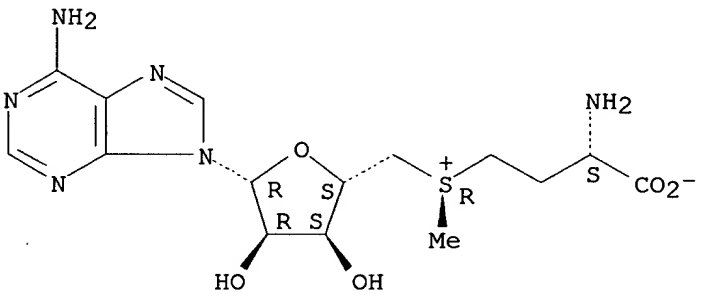
AB The substrate stereospecificity of 1-aminocyclopropane-1-carboxylate synthase (I), a pyridoxal phosphate-containing enzyme, from the pericarp tissue of tomatoes was studied using the various stereoisomers of S-adenosylmethionine (II) at both the sulfonium pole and the amino acid center. The data indicated that only the naturally occurring isomer (-)-L-II acts as substrate (Km = 20 μM). Both (±)-D-II and (+)-L-II were inactive as substrates. (+)-L-II (Ki = 15 μM) was a potent inhibitor of I, whereas (±)-D-II (Ki = 70 μM) was less active as an inhibitor. This active isomer had the (S) configuration at both the S and the α-C atoms of the amino acid portion of II.

IT **91279-78-6**
RL: BIOL (Biological study)
(aminocyclopropanecarboxylate synthase inhibition by, kinetics of, enzyme stereospecificity in relation to)

RN 91279-78-6 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1982:402764 CAPLUS
DOCUMENT NUMBER: 97:2764
TITLE: Isotopic mapping of transition-state structural features associated with enzymic catalysis of methyl transfer
AUTHOR(S): Rodgers, James; Femec, Douglas A.; Schowen, Richard L.
CORPORATE SOURCE: Dep. Chem., Univ. Kansas, Lawrence, KS, 66045, USA
SOURCE: Journal of the American Chemical Society (1982), 104(12), 3263-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In order to compare the mol. structures of nonenzymic and enzymic S-to-O transmethylation transition states by the use of kinetic isotope effects, a series of isotopic maps was produced. In these, contours of constant isotope effect were displayed vs. the Pauling bond orders BCS and BCO, for the C-S and C-O bonds, resp., taken as independent variables to describe the transition states. Maps were calculated with the BEBOVIB computer program for k(CH3)/k(CD3), k(12CH3)/k(13CH3), k(16O)/k(18O), and k(32S)/k(34S), with 2 models for the reaction coordinate, 2 force-field assumptions, and

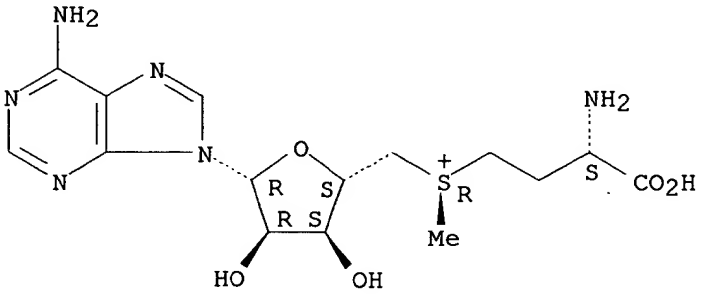
4 temps. Nonenzymic isotope effects and isotope effects for catechol O-methyltransferase action were then used to construct figures on the (CH3/CD3) and (12CH3/13CH3) maps which corresponded to allowed spaces of transition-states structures. Superposition of the figures yielded the spaces of transition-state structures simultaneously consistent with both H and C isotope effects. It was concluded that the enzyme compresses the SN2 transition state and that the compression of the C-O and C-S bonds may well be of the order of 0.15 Å/bond and could conceivably be more than twice as large.

IT **60018-86-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyltransferases, transition-state structure in)

RN 60018-86-2 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1981:551125 CAPLUS

DOCUMENT NUMBER: 95:151125

TITLE: S-adenosyl-L-methionine and S-adenosyl-L-homocysteine, an NMR study

AUTHOR(S): Stolowitz, Mark L.; Minch, M. J.

CORPORATE SOURCE: Chem. Dep., Univ. Pac., Stockton, CA, 95211, USA

SOURCE: Journal of the American Chemical Society (1981), 103(20), 6015-19
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

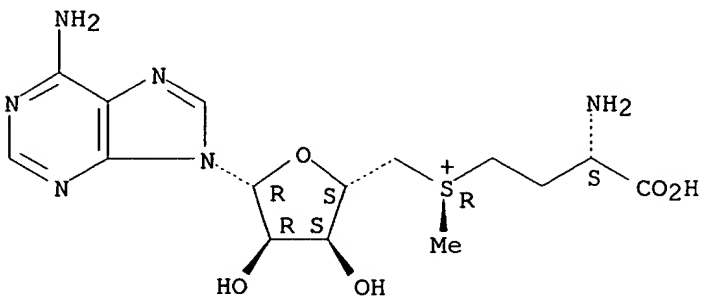
AB The conformations of the title compds. (I and II, resp.) were determined from their 360-MHz 1H NMR in D2O. The ribose of both compds. has a C3'-exo conformation, but I has 1 favored gauche-anti conformation about the C4'-C5' bond, whereas the orientation about the C4'-C5' bond of II is distributed between 2 gauche-anti rotamers. The methionine side chain of I undergoes rapid rotation about the Cα-Cβ and Cβ-Cγ bonds, whereas the side chain of II has a preference for the gauche-anti conformations about the Cα-Cβ bond. The 1H and 13C NMR of com. available (-)-I indicated the presence of a small amount of the (+)-sulfonium diastereomer.

IT **79297-26-0 79297-28-2 79297-30-6**
RL: PRP (Properties)
(NMR of)

RN 79297-26-0 CAPLUS

CN Adenosine, 5'-[(3-amino-3-carboxypropyl)methylsulfonio]-5'-deoxy-, iodide, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

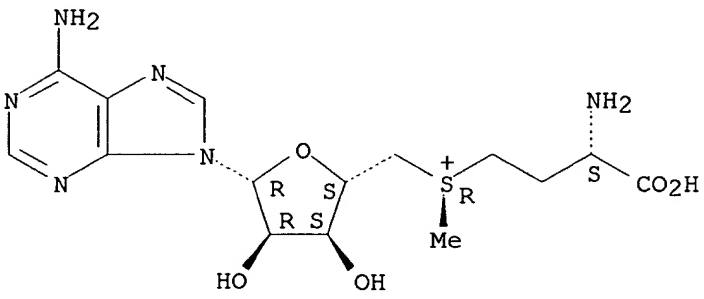
Absolute stereochemistry.



● I^-

RN 79297-28-2 CAPLUS
CN Adenosine, 5'-[(3-amino-3-carboxypropyl)methylsulfonio]-5'-deoxy-, chloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



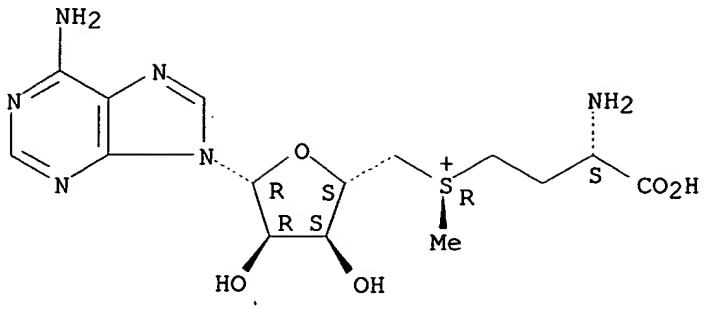
● Cl^-

RN 79297-30-6 CAPLUS
CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy-, sulfate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

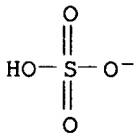
CRN 60018-86-2
CMF C15 H23 N6 O5 S

Absolute stereochemistry.

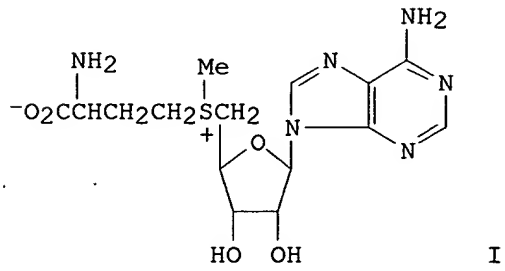


CM 2

CRN 14996-02-2
CMF H O4 S



L3 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1976:487099 CAPLUS
DOCUMENT NUMBER: 85:87099
TITLE: Potential inhibitors of S-adenosylmethionine-dependent methyltransferases. 5. Role of the asymmetric sulfonium pole in the enzymic binding of S-adenosyl-L-methionine
AUTHOR(S): Borchardt, R. T.; Wu, Yih Shiong
CORPORATE SOURCE: Dep. Biochem., Univ. Kansas, Lawrence, KS, USA
SOURCE: Journal of Medicinal Chemistry (1976), 19(9), 1099-103
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB For the transmethylations catalyzed by catechol O-methyltransferase (EC 2.1.1.6) [9012-25-3], phenylethanolamine N-methyltransferase (EC 2.1.1.28) [9037-68-7], histamine N-methyltransferase (EC 2.1.1.8) [9029-80-5], and hydroxyindole O-methyltransferase (EC 2.1.1.4) [9029-77-0], the natural enantiomer 10(-)-S-adenosyl-L-methionine[(-)-SAM][(-)-I] was active as a Me donor, while 903 (+)-SAM was inactive. (+)-SAM, prepared by enzymic resolution of (±)-SAM [23095-97-8], was a potent inhibitor of the enzyme-catalyzed transmethylations. The relation of configuration to enzyme binding and methyl transfer was discussed.

IT **60018-86-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and methyltransferase binding by)

RN 60018-86-2 CAPLUS

CN Adenosine, 5'-[(R)-[(3S)-3-amino-3-carboxypropyl]methylsulfonio]-5'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.